

Phosphonic acid, bis(1-methylethyl) ester  
1809-20-7 | DTXSID7061988

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -64.3 °C

Global applicability domain: Inside

Local applicability domain index: 5.71e-01

Confidence level: 7.25e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Triethyl phosphate</div> <div>Measured: -56.4</div> <div>Predicted: -54.1</div>	<div>Image not found</div> <div>Tributyl phosphate</div> <div>Measured: -79.0</div> <div>Predicted: -70.4</div>	<div>Image not found</div> <div>Dimethyl hydrogen phosphite</div> <div>Measured: -60.0</div> <div>Predicted: -61.6</div>
<div>Image not found</div> <div>Tributyl phosphite</div> <div>Measured: -80.0</div> <div>Predicted: -73.8</div>	<div>Image not found</div> <div>Trimethyl phosphate</div> <div>Measured: -46.0</div> <div>Predicted: -49.9</div>	